

W0031

Lattice-dynamical Modelisation of Physical Properties of Crystals. Carlo Maria Gramaccioli, Univ. of Milan, Dept. of Earth Sciences, Milan, Italy.

Among the various kinds of modeling crystal structures, particularly interesting is the possibility of deriving physical properties depending upon the vibrational behaviour. Such a perspective is linked to the success of empirical atom-atom potentials in reproducing the vibrational modes with good approximation using lattice dynamics.

Besides vibrational frequencies, thermodynamic functions at different temperatures, such as specific heat, entropy, free energy, etc., can be evaluated; this successful performance concerns both molecular and ionic crystals, including complex cases such as the most common silicate minerals.

For crystallography, a promising application is that of reproducing atomic displacement parameters (ADP's) and correcting the bond distances for thermal motion. Although such a procedure involves complex calculations, nevertheless it affords important evidence in interpreting the atomic and molecular motion, even for complex cases when molecules are not entirely rigid.

Examples of applications of the above mentioned procedures are given in this presentation.